Chapter 9

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1 Boltzmann Transport Equation

To get a firmer grasp on GMR, we need a more powerful way to model resistance in metals. Therefore, we need to be able to calculate the current density j that results from an electric field $\mathcal{E}$, $j = \sigma\mathcal{E}$ (Ohm's law). In the free-electron gas model of a metal, we can sum the charge flux $e \cdot v_x$ in a direction x over all states:

$$j = \frac{-e}{(2\pi)^3} 2 \int f(k) v_x(k) d^3k \tag{1}$$

where the 2 is for spin degeneracy and the volume integral is over all k-space. In the absence of an electric field, the distribution function is the Fermi-Dirac

$$f(k) = f_0(k) = \frac{1}{e^{(E(k)-E_F)/k_B T} + 1} \tag{2}$$

where the subscript on f_0 denotes equilibrium. As usual, $E(k) = \frac{\hbar^2 k^2}{2m}$. This function is symmetric under reflection in the x direction, but $v_x(k) = \frac{\hbar k_x}{m}$ clearly is not. Therefore, the integral of the product of these odd and even functions over the symmetric bounds is zero. This is to be expected, since no net current flows in the absence of an electric field.

When an electric field is imposed, the distribution function must be pushed out of equilibrium, resulting in a net current upon integration of the above expression. We can write

$$f(k) = f_0(k) + g(k) \tag{3}$$

Since the first term contributes nothing to the current, our task is then to calculate $g(k)$. The Boltzmann Transport Equation (BTE) gives us this.

Our task to model GMR is to investigate the BTE for

1. 3-D bulk metal transport
2. Thin film metal transport
3. Ferromagnetic metal transport

Before tying everything together (ferromagnetic multilayer) in GMR.

1.1 3-D bulk transport

The BTE is a statement of steady-state. There is a rate of excitation and a rate of relaxation. In steady-state, these two rates are equal.

$$\frac{df}{dt}\Big|_{excitation} = \frac{df}{dt}\Big|_{relaxation} \tag{4}$$

The RHS is simple to express. Using the relaxation rate approximation, we introduce a phenomenological relaxation time τ over which the electron gas regains equilibrium:

$$\frac{df}{dt}\Big|_{relaxation} = \frac{f - f_0}{\tau} = \frac{g}{\tau} \tag{5}$$

The LHS is due to an electric field (in, say, the x direction), which provides an electrostatic force $e\mathcal{E}$ on the electrons. We therefore decompose the derivative:

$$\frac{df}{dt}\mid_{excitation}=\frac{df}{dp_x}\frac{dp_x}{dt}=\frac{df}{dp_x}Force=\frac{df}{dk_x}\frac{e\mathcal{E}}{\hbar} \tag{6}$$

Now, because $k^2 = k_x^2 + k_y^2 + k_z^2$, we can write

$$dk_x = \frac{k}{k_x}dk \tag{7}$$

giving

$$\frac{df}{dt}\mid_{excitation}=\frac{df}{dk}\frac{e\mathcal{E}}{\hbar}\frac{k_x}{k} \tag{8}$$

The BTE then says

$$g = \frac{df}{dk}\frac{e\mathcal{E}}{\hbar}\frac{k_x}{k}\tau \tag{9}$$

Now, we can use this expression to calculate the current associated with the electric field:

$$j = \frac{-e}{(2\pi)^3}2\int g(k)\frac{\hbar k_x}{m}dk^3 \tag{10}$$

$$j = \frac{-2e}{(2\pi)^3}e\mathcal{E}\tau\int\frac{df}{dk}\frac{k_x^2}{k}d^3k \tag{11}$$

At temperatures $k_BT << E_F$, the distribution function $f(k)$ is unity inside the Fermi sphere and zero outside. Therefore, $\frac{df}{dk} \approx -\delta(k-k_F)$. This converts the volume integral into an integral over the Fermi surface.

$$j = \frac{1}{4\pi^3}\frac{e^2\tau}{m}\mathcal{E}\int_{Fermi}\frac{k_x^2}{k}dS \tag{12}$$

Now transform to spherical coordinates:

$$k_x = k_F\cos\phi\sin\theta \tag{13}$$

$$dS = k_F^2\sin\theta d\theta d\phi \tag{14}$$

$$\int\frac{k_x^2}{k}dS = k_F^3\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin^3\theta\cos^2\phi = \frac{4\pi}{3}k_F^3 \tag{15}$$

$$j = \frac{e^2\tau}{m}\mathcal{E}\frac{v_F^3}{3\pi^2} \tag{16}$$

Now, since the electron density is

$$n = \frac{2}{(2\pi)^3}\int_0^{k_F}d^3k = \frac{2}{(2\pi)^3}\frac{4\pi}{3}k_F^3 = \frac{k_F^3}{3\pi^2} \tag{17}$$

we have

$$j = \frac{e^2n\tau}{m}\mathcal{E} \tag{18}$$

This you should recognize as Ohm's law $j = \sigma\mathcal{E}$, with a conductivity equal to precisely the expression we calculated within the classical Drude model.

2 Fuchs-Sondheimer model

Consider now a metallic thin film with an electric field $\mathcal{E}_x$. The thickness of the film (in the z-direction) is t.

When we lose the translational invariance in bulk conductors by using thin films, we have to take this into account by using the full time derivative of the electron momentum distribution in the Boltzmann equation:

$$\frac{df}{dt}\mid_{relaxation}=\frac{dg}{dz}\frac{dz}{dt}+\frac{g}{\tau}=\frac{e\mathcal{E}}{m}\frac{df_0}{dv_x} \tag{19}$$

The first term is called the convective derivative and can be rewritten $v_z\frac{dg}{dz}$. Clearly, this term (and its x and y counterparts) is zero in the bulk case because g does not depend on any spatial variable when full translational symmetry is present. This equation has the solution

$$g=\frac{e\mathcal{E}\tau}{m}\frac{df}{dv_x}\left[1+F(v)e^{-\frac{z}{v_z\tau}}\right]. \tag{20}$$

where $F(v)$ is determined by boundary conditions. Since the sign of v_z changes at either boundary (at $z=0$ and $z=t$), we must break up the solution into two pieces: one for the distribution traveling up and the other traveling down:

$$g^+=\frac{e\mathcal{E}\tau}{m}\frac{df}{dv_x}\left[1-F^+e^{-\frac{z}{v_z\tau}}\right]. \tag{21}$$

$$g^+=\frac{e\mathcal{E}\tau}{m}\frac{df}{dv_x}\left[1-F^-e^{-\frac{t-z}{v_z\tau}}\right]. \tag{22}$$

The F^+ and F^- coefficients are determined by the boundary conditions. We assume diffusive scattering, meaning strong relaxation at the boundaries imposes

$$g^+(z=0)=0 \tag{23}$$
$$g^-(z=t)=0 \tag{24}$$

This determines the coefficients, $F^-=F^+=-1$.

Now we can determine the current flowing in the film, with the usual expression:

$$j=-\frac{e}{4\pi^3}\int f(k,z)v_x(k)dk \tag{25}$$

where $f(v,z)=[g^+(v,z)+g^-(v,z)]$. We again use spherical coordinates, and the $\frac{df_0}{dk}$ term reduces the volume integral to one over the sphere of radius k_F. We also remember that since we have broken up our solution to $v_z>0$ and $v_z<0$ cases and $v_z=\frac{\hbar k_F}{m}cos(\theta)$ in spherical coordinates, g^+ is integrated only over the $\theta=0..\pi/2$ hemisphere, and g^- is integrated over the remainder. After doing the trivial integration of $cos^2(\phi)$, we have

$$j(z)=\frac{e^2\mathcal{E}\tau}{4\pi^2 m}k_F^3\left[\int_0^{\pi/2}sin^3\theta\left(1-e^{\frac{-z}{\lambda cos\theta}}\right)d\theta+\int_{\pi/2}^{\pi}sin^3\theta\left(1-e^{\frac{-(t-z)}{\lambda cos\theta}}\right)d\theta\right] \tag{26}$$

where $\lambda=\frac{\hbar k_F}{m}\tau$ is the mean free path. We can combine these two integrals into one with the same bounds and simplify using

$$e^{-z}+e^{-(t-z)}=2e^{-t/2}cosh(\frac{t-2z}{2}), \tag{27}$$

giving

$$j(z)=2\frac{e^2\mathcal{E}\tau}{4\pi^2 m}\frac{k_F^3}{3\pi^2}3\pi^2\int_0^{\pi/2}sin^3\theta\left[1-e^{\frac{-t}{2\lambda cos\theta}}cosh(\frac{t-2z}{2\lambda cos\theta})\right]d\theta \tag{28}$$

Now, since this is a function of z (i.e. the current density is different near the boundaries) we need to average over the cross-section:

$$j=\frac{1}{t}\int_0^t j(z)dz=\sigma_0\mathcal{E}\left[1-\frac{3\lambda}{2t}\int_0^{\pi/2}sin^3\theta\cos\theta\left(1-e^{\frac{-t}{\lambda cos\theta}}d\theta\right)\right] \tag{29}$$

where σ_0 is the Drude conductivity, $\frac{e^2\tau n}{m}$. By making the variable substitution $\chi = 1/cos\theta$, this integral can be re-written as

$$j = \sigma_0 \mathcal{E}\left[1 - \frac{3\lambda}{2t}\int_1^\infty \left(\frac{1}{\chi^3} - \frac{1}{\chi^5}\right)\left(1 - e^{-\frac{t}{\lambda}\chi}\right) d\chi\right] \tag{30}$$

For a thick film, $\lambda << t$ and $e^{-\frac{t\chi}{\lambda}} \to 0$. Then we can do either form of the integral analytically and

$$j \approx \mathcal{E}\sigma_0 \left[1 - \frac{3\lambda}{8t}\right] \tag{31}$$

For a thin film, $\lambda >> t$ and the result is

$$j \approx \mathcal{E}\sigma_0 \frac{3}{4}\frac{t}{\lambda} \ln\frac{\lambda}{t} \tag{32}$$

These results assume perfectly diffusive scattering at the boundaries. If the scattering is instead partially specular with fraction p, then the thick film limit is

$$\frac{\sigma}{\sigma_0} = 1 - \frac{3\lambda}{8t}(1-p) \tag{33}$$

which reduces to the bulk conductivity when the scattering is perfectly specular. This makes sense because perfectly specular reflecting boundaries are tantamount to periodic boundary conditions, repeating the film on both sides and extending the effective thickness to infinity.

3 Boltzmann Equation for Ferromagnetic Metals

For ferromagnets we have to solve two equations, one for each spin species. In each equation we must include the scattering time as we have done before, but in general these will be different for each spin. In addition, we must also account for relaxation of spin up (down) into spin down (up) over the spin relaxation time $\tau_{\uparrow\downarrow}$:

$$\frac{df_0}{dE}v_x e(E) = \frac{g_\uparrow}{\tau_\uparrow} + \frac{g_\uparrow - g_\downarrow}{\tau_{\uparrow\downarrow}} \tag{34}$$

$$\frac{df_0}{dE}v_x e(E) = \frac{g_\downarrow}{\tau_\downarrow} + \frac{g_\downarrow - g_\uparrow}{\tau_{\uparrow\downarrow}} \tag{35}$$

These are two linear equations with two unknowns. The solutions for $g_\uparrow$ and $g_\downarrow$ are readily found with some algebra:

$$\frac{df_0}{dE}v_x e(E) = \left[\frac{(\frac{1}{\tau_\uparrow} + \frac{1}{\tau_\downarrow})\frac{1}{\tau_{\uparrow\downarrow}} + \frac{1}{\tau_\uparrow\tau_\downarrow}}{\frac{1}{\tau_\downarrow} + \frac{2}{\tau_{\uparrow\downarrow}}}\right] g_\uparrow \tag{36}$$

and

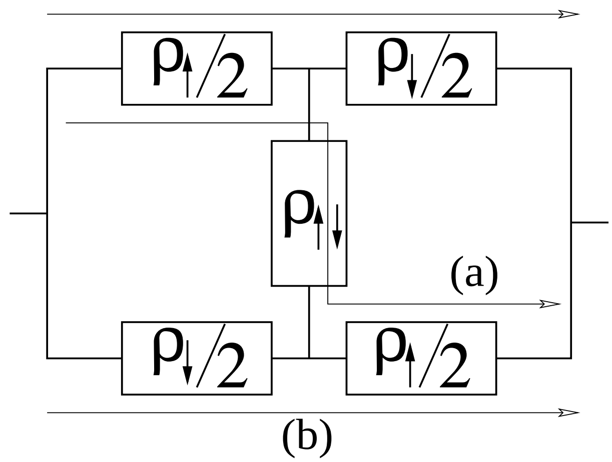
$$\frac{df_0}{dE}v_x e(E) = \left[\frac{(\frac{1}{\tau_\uparrow} + \frac{1}{\tau_\downarrow})\frac{1}{\tau_{\uparrow\downarrow}} + \frac{1}{\tau_\uparrow\tau_\downarrow}}{\frac{1}{\tau_\uparrow} + \frac{2}{\tau_{\uparrow\downarrow}}}\right] g_\downarrow \tag{37}$$

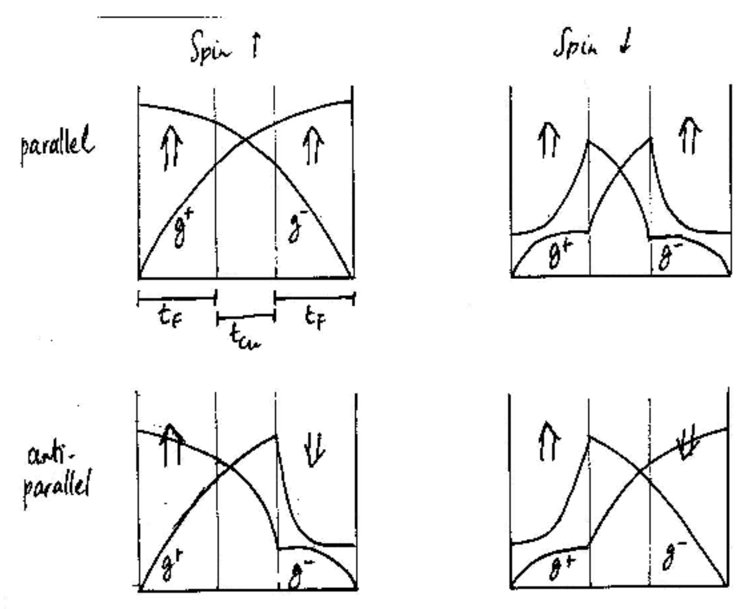
This is just like the Fuchs-Sondheimer Boltzmann equation, except now $\frac{1}{\tau}$ is replaced with the term in brackets. Since this term does not depend on k, we can skip to the last step of the determination of the conductivity:

$$\sigma = \sigma_\uparrow + \sigma_\downarrow = \frac{ne^2}{m}\left[\frac{\frac{1}{\tau_\uparrow} + \frac{1}{\tau_\downarrow} + \frac{4}{\tau_{\uparrow\downarrow}}}{\frac{1}{\tau_\uparrow\tau_\downarrow} + \frac{1}{\tau_{\uparrow\downarrow}}(\frac{1}{\tau_\downarrow} + \frac{1}{\tau_{\uparrow\downarrow}})}\right] \tag{38}$$

This is equivalent to a resistor network shown in the figure, where as usual $\rho \propto \frac{1}{\tau}$. For small $\rho_{\uparrow\downarrow}$, most of the current passes through path a corresponding to weak spin mixing. For a large $\rho_{\uparrow\downarrow}$, current must pass through path b, corresponding to strong spin mixing.

4 Boltzmann Results for GMR


ρ↑/2
ρ↓/2
ρ↑↓
(a)
ρ↓/2
ρ↑/2
(b)


Spin ↑
Spin ↓
parallel
anti-
parallel
g+
g-
tF
tCu
tF